PERGAMON

International Journal of Rock Mechanics & Mining Sciences 38 (2001) 1–4

International Journal of Rock Mechanics and Mining Sciences

www.elsevier.com/locate/ijrmms

Foreword

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Accepted 24 August 2000

In countries where radioactive waste is produced, disposal in underground repositories has become the most attractive design option for permanent isolation of spent fuel and other radioactive wastes. To evaluate the various geological media and sites considered for such disposal, we must characterize different host rocks and study alternative repository designs at the different sites. An important part of the performance and safety assessment of the disposal system is to incorporate the coupling of mechanical stability, groundwater flow through the repository, and thermal loading from the decaying waste.

To help meet these objectives and provide the theoretical background for performance and safety assessment, we aim to develop models capable of simulating coupled thermo–hydro–mechanical (T–H–M) processes. The term 'coupled processes' implies that one process affects the initiation and progress of another. Thus, the response of a rock mass to radioactive waste storage cannot be predicted with confidence by considering each process individually or in direct succession. In the field of rock mechanics, the main focus of studies has been on the specific binary couplings T–M and H–M. In recent years, interest has been focused on the full triple T–H–M coupling. In the future, we can foresee the introduction of chemical processes (C) and, in turn, the study of T–H–M–C coupling.

The coupling of T–H–M processes is a major challenge to the science community, since the three processes have widely different characteristic time and spatial scales. The thermal gradient for rock material has relatively large time and spatial scales. Mechanical effects, on the other hand, have a short time scale, since changes in the mechanical response can propagate through the rock mass with the speed of sound and the deformability is controlled mainly by the presence of large discontinuities, such as faults and shear zones. Finally, groundwater flow and transport are sensitive to small-scale heterogeneities and are characterized by large flow and solute transport times.

Numerically, these processes can be modelled by different techniques, such as finite-difference methods, finite-element methods, and discrete-element methods. In addition, many of the coupled processes are non-linear, and the constitutive equations typically contain large parameter sets. To combine all these processes into an efficient model for the simulation of coupled T–H–M processes in fractured rocks is not an easy task.

Another aim for the study of coupled T–H–M processes is to be able to verify numerical codes and validate model results against well-conditioned field and laboratory experiments. Here, the challenge lies in providing a set of well-defined conditions for the boundaries, rates of thermal and mechanical loading, initial state of stress, temperature and flow, constitutive equations, methods of coupling, and material properties. Coupled T–H–M experiments in the field require well-planned test design and careful instrumentation. They often have durations of months and years, and are very costly.

This Special Issue deals with the major results from the second phase of the international cooperative research project DECOVALEX II which took place from November 1995 to June 1999. (DECOVALEX is an acronym for DEvelopment of COupled models and their VALidation against EXperiments in nuclear waste isolation.) The content of the Special Issue demonstrates some of the progress made on coupled processes modeling since the presentation of the previous Special Issue of this Journal in 1995 (on results obtained from the first phase of the DECOVALEX project, 1992–1996, i.e., DECOVALEX I).

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1365-1609/01/$ - see front matter
PII: S1365-1609(00)00059-9

The overall objective of the DECOVALEX project is to increase the understanding of various T–H–M processes of importance for radionuclide release and transport from a repository to the biosphere, and how the processes can be described by mathematical models. In the DECOVALEX I project, a number of hypothetical benchmark tests and small laboratory test cases were studied, as well as some larger-scale in-situ experiments. At the end of this first phase, we decided to alter the focus to two major large-scale in-situ experiments. Further, an additional objective of the project was to evaluate how the studies conducted in the project can be applied to the safety and performance assessment of a potential repository.

Within these overall objectives, four tasks were defined for the DECOVALEX II project:

Task 1: Numerical study of Nirex's Rock Characterization Facility (RCF) shaft excavation at Sellafield, UK — simulation of the coupled hydro-mechanical processes of the RCF pumping test and responses of the rock mass to the shaft excavation, including the excavation disturbed zone (EDZ).

Task 2: Numerical study of PNC's in situ T–H–M experiments in Kamaishi Mine, Japan — an integrated investigation of a complete rock–buffer–heater system under in-situ conditions over a long period of time.

Task 3: Review of the state-of-the-art of the constitutive relations of rock joints.

Task 4: A report on the current understanding of the coupled T–H–M processes related to design and performance assessment of radioactive waste repositories.

The results of Tasks 1, 2, and 4 are presented in this Special Issue. Representatives of 12 Funding Organizations from seven countries formed the Steering Committee of the project, and 11 Research Teams participated in DECOVALEX II. Progress and results were reported and discussed at five Workshops and four Task Force meetings.

Descriptions of the tasks are presented below and the resultant papers forming Parts A, B and C of this Special Issue are introduced.

Part A: Prediction of the hydro-mechanical response during shaft sinking of the proposed Nirex RCF Facility near Sellafield, Cumbria County, UK

The coupled H–M responses in the fractured volcanic rocks of the Borrowdale Volcanic Group at Sellafield to a long-term pumping test and the proposed shaft sinking phase of Nirex's Rock Characterization Facility were studied by six research teams. The work was divided into three subtasks. The first subtask undertaken was a blind prediction of the hydraulic response of a pumping test in a well, labeled RCF3, at the location of one of the planned shafts. The test comprised of an abstraction phase of 2,110 h that gave a drawdown of 158 m at the level 640–680 m below sea level, followed by a recovery phase of 718 h. Teams were asked to predict the transient flow rate in the abstraction zone and the pressure responses of 18 monitoring zones in adjacent boreholes. The research teams were free to derive their own conceptual models of the hydrogeology in the test area, as well as select boundary conditions and material properties based on the vast background material provided by Nirex. Large discrepancies between the predictions of individual research teams and between predictions and observed responses were obtained.

In the next subtask, data on the responses at the initial set of 18 monitoring zones were released to research teams for calibration and redefinition of their conceptual models. Following calibration, the teams made new predictions for 16 other monitoring zones, and results were presented according to a given protocol. The results showed acceptable predictions for initial and final pressures in the monitoring zones and significant improvements in the measurements of transient behavior. The final outcome of the subtask was establishing that the calibrated models were capable of representing steady-state conditions, but transient conditions were not well simulated. To some extent, this may be an artifact of the calibration process, which focused on the pressure responses — rather than transient flow behavior.

After having gained experience in the analysis of the hydrogeological response to the RCF3 pump test, the research teams were asked to predict the H–M response of sinking a shaft along the axis of the same borehole for a depth interval of 640–680 m below sea level at Sellafield. The teams were asked to model water inflow, groundwater pressure response, rock mass displacement, convergence and stress changes in the vicinity of the shaft wall. They were then asked to determine the extent of the EDZ and of reinforcement needed to stabilize the shaft. All the teams predicted small initial and steady-state inflow to the shaft and small radial displacements in the directions of the in-situ principal stresses. Part way through the course of study, Cumbria County Council rejected the planning application by NIREX and the shaft sinking at the Sellafield site was not carried out. Hence, the predictions could not be evaluated against real data.

The task is unique in DECOVALEX to date in that an extensive data package was distributed to research teams who were free to select, develop, and parameterize their own conceptual models of the Sellafield site. This was to ensure that a truly independent analysis could be performed. The background and objectives of the studied task and a brief summary of the results by the research teams and major scientific and logistical lessons learned are presented by Knight in the first paper. This is followed by four further papers covering the Sellafield work. A range of models was devised for the task, that varied in their partition of flow between the faults and the remainder of the fracture network (discrete-fracture network models) or between faults and matrix (equivalent continuum models). The discrete fracture network approach is used in the second paper, by Rejeb and Bruel. A stochastic model of the 3D fractured rock is used by Gomez-Hernandez and co-workers (the third paper) to analyze the flow response of the system, while the continuum approach is used by Kobayashi (the fourth paper which presents theory and results of the full hydromechanical coupling of the problem) and Hakami (the fifth paper). It is useful and instructive to see results of these alternative and perhaps complementary approaches to address the same task.

Much has been learned from efforts on this task. One particular outcome is that the importance of a prediction – calibration procedure in predicting the response to pumping and shaft sinking in this type of modeling has become evident, and how to properly perform such a procedure in a real site-scale problem is an interesting issue. Another conclusion from the work under this task is that treating hydrological and mechanical processes as fully coupled processes remains significantly more difficult under realistic in situ conditions than treating the processes separately.

Part B: Numerical study of the Kamaishi Mine In Situ T–H–M experiments

The Kamaishi Mine Heater Test (see cover of this Special Issue) was an experiment conducted in a $5 \times 7\,\mathrm{m}^2$ alcove excavated from an existing drift located at a depth of about 250 m. In 1995, a vertical test pit, 1.7 m in diameter and 5 m in depth, was drilled in the floor of the alcove. The hole was drilled with a gentle shot boring method, using a large-diameter boring machine to avoid mechanical disturbance of the rock. In 1996, an electric heater was installed into the test pit and surrounded by a buffer of bentonite clay. Bentonite was placed into the test pit in layers of 0.5 m, with compaction of each layer to a dry density of about $1.6\,\mathrm{ton/m^3}$. After the entire test pit was filled with bentonite, a watertight concrete lid was placed on the drift floor, which in turn was supported by steel bars from the ceiling of the drift. Because the rock was not fully saturated immediately around the test pit, a flooding pool was set up on the drift floor above the test pit. At the end of 1996, the heater was turned on and the temperature was set to 100°C for 8.5 months, followed by a 6-month cooling period. System responses, including temperature, moisture content, fluid pressure, stress, strain and displacement, were measured in both the bentonite and surrounding rock mass. The experiment was completed in early 1998, and thereafter the monitoring sensors were recovered and re-calibrated.

The task for the DECOVALEX research teams was to predict the T–H–M effects in the buffer material inside the test pit and in the surrounding rock, both during excavation of the test pit and the heater testing. The test case was divided into three main tasks: Tasks 2A, 2B and 2C. Task 2A was to predict the H–M effects in the rock caused by the excavation of the test pit. Geometrical, mechanical and hydraulic rock properties, and hydraulic conditions before excavation were given to the research teams, and they were asked to predict water inflow distribution in the test pit. Task 2B was a model calibration of rock and fracture properties and the hydromechanical boundary conditions, based on actual measured results which were predicted in Task 2A. Task 2C was to predict the T–H–M effects in the rock and buffer during the heating experiment. The rock model was presumed to have properties based on the calibration in Task 2B, with correct permeability distribution in the near-field rock. At every step, all the model predictions were made before completion of the respective test and before the experimental data were presented. Thereafter, the model results were compared with the experimental results, as well as with the modeling results of other research teams within the DECOVALEX project.

Processes being studied in the modeling of the Kamaishi Test include groundwater and heat flow in the rock matrix, fractures, buffer and their interfaces under varying unsaturated conditions. Prior to the emplacement of buffer and heater, the inflow of water into the test pit is affected, not only by the presence of fractures, but also by the unsaturated condition of the rock near the test pit. Strong variation in the areal distribution of inflow was observed on the walls of the test pit. After the heater and bentonite were emplaced, diffusion of water into the bentonite from the rock occurred simultaneously with drying of the bentonite near the heater. The multiphase flow in the bentonite region with phase transition gives rise to a varying swelling or shrinking across the bentonite region. Such deformation interacts with the rock permeability, with open questions concerning the flow processes in the interface between the rock and the buffer. The coupled T–H–M processes under such varying saturation conditions are complex and are at the leading edge of our modeling capabilities.

A full description of the Kamaishi experiment, main results and T–H–M behavior of the system is presented by Chijimatsu et al. in the first paper of

Part B. Nguyen et al. discuss their work in the next paper on predicting H–M effects on water inflow into the test pit excavated in the fractured rock, including the effects of unsaturated conditions near the pit walls. Börgesson and co-workers have also contributed a paper describing the model studies of the DECOVALEX project teams on a series of laboratory tests on bentonite materials. Finally, Rutqvist et al. in the last two papers of Part B, review the T–H–M theories and numerical formulations for partially saturated rocks and present a comparative review of the coupled T–H–M analyses by the DECOVALEX teams on the Kamaishi experiment. Lessons learned and further development needs, both in modeling and in test and measurement design, are also discussed.

The Kamaishi Mine heater test has provided valuable experience in analyzing coupled T–H–M processes for a problem similar to that posed by a real nuclear waste repository. In the course of the DECOVALEX II project, each research team contributed and learned from the others, and new modeling capabilities in simulating unsaturated T–H–M processes within rock-bentonite-heater systems were developed, tested, and applied.

Part C: Coupled T–H–M issues relating to radioactive waste repository design and performance assessment

This task of DECOVALEX II considered the T–H–M information and outlined the current state-of-knowledge on coupled T–H–M issues related to nuclear waste repository performance. The results are summarized in the paper by Hudson et al. — which includes sections on the T–H–M background, the interface with performance assessment (PA) including the role of T–H–M issues in the overall repository design context, and the nature of numerical codes and how the content of the codes can be audited. Also, state-of-knowledge statements elicited at a series of DECOVALEX II workshops are presented.

The above descriptions introduce this Special Issue which brings together results, information, and data that emerged from the efforts of the research teams of the DECOVALEX II co-operative project. Although our capability in modeling coupled T–H–M processes is still at an early stage of development, we have reached the point where we feel confident that our codes and models in principle reflect the behavior of the real rock mass and the engineering backfill.

The major advance that DECOVALEX II has helped to bring about is the development of coupled models to simulate the response of the highly compacted unsaturated bentonite to the coupled processes of heat and resaturation and the mechanical response of the rock mass. In the next phase of the DECOVALEX project, DECOVALEX III, modeling will be applied to the large-scale buffer mass experiment FEBEX at the Grimsel test site in Switzerland and the Drift Scale Heater Test in Yucca Mountain at the Nevada Test Site. In addition, three benchmark tests related to resaturation, upscaling, and glaciation will be performed together with a more general study of the importance of coupled T–H–M processes for safety and performance assessment in radioactive waste isolation.

We would like to take this opportunity to express our appreciation to the Funding Organizations of the DECOVALEX II project for their continuing support and encouragement and to all the Research Teams for their conscientious work, open discussions and cooperative attitudes, that have made the project a success. We would also like to thank John Hudson, Editor-in-Chief of the IJRMMS, for his agreement and help in preparing this Special Issue.